



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID : 3AFE / pdb_00003afe
Title : Crystal structure of the HsaA monooxygenase from M.tuberculosis
Authors : D'Angelo, I.; Lin, L.Y.; Dresen, C.; Tocheva, E.I.; Eltis, L.D.; Strynadka, N.
Deposited on : 2010-02-28
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

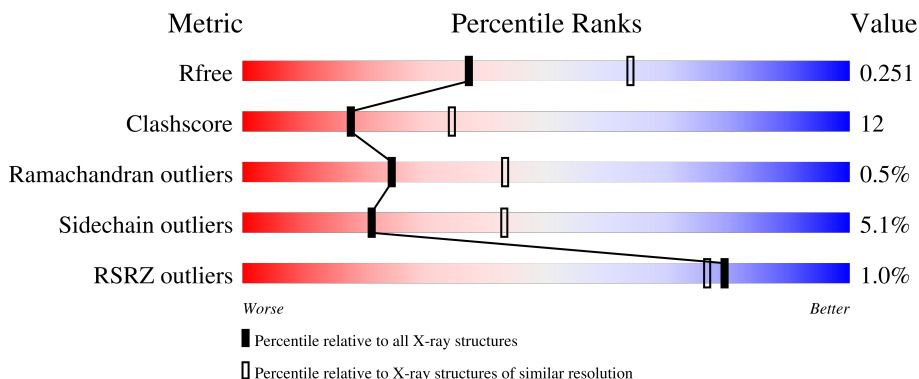
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	394	
1	B	394	
1	C	394	
1	D	394	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12261 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hydroxylase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2970	1877	537	547	9			
1	B	379	Total	C	N	O	S	0	0	0
			2935	1853	531	542	9			
1	C	381	Total	C	N	O	S	0	0	0
			2948	1860	533	546	9			
1	D	379	Total	C	N	O	S	0	0	0
			2936	1855	532	541	8			

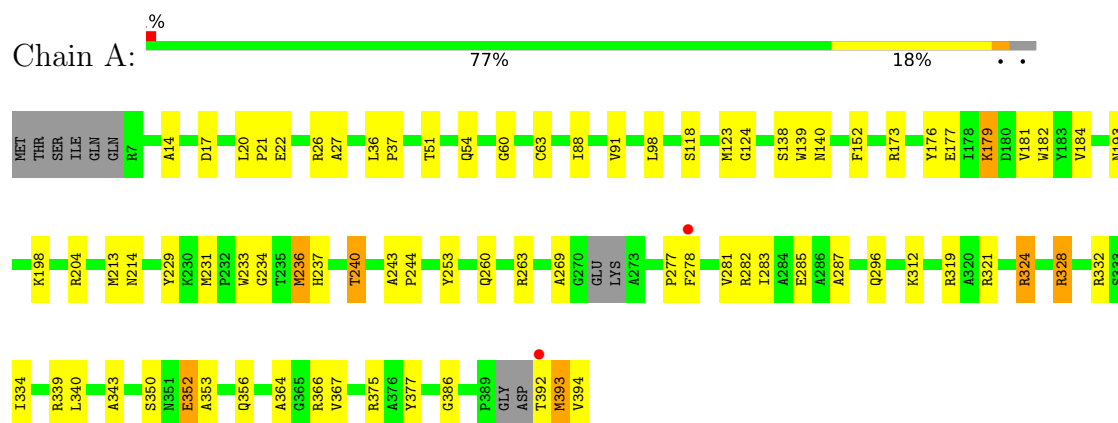
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	158	Total	O	0	0
			158	158		
2	B	114	Total	O	0	0
			114	114		
2	C	90	Total	O	0	0
			90	90		
2	D	110	Total	O	0	0
			110	110		

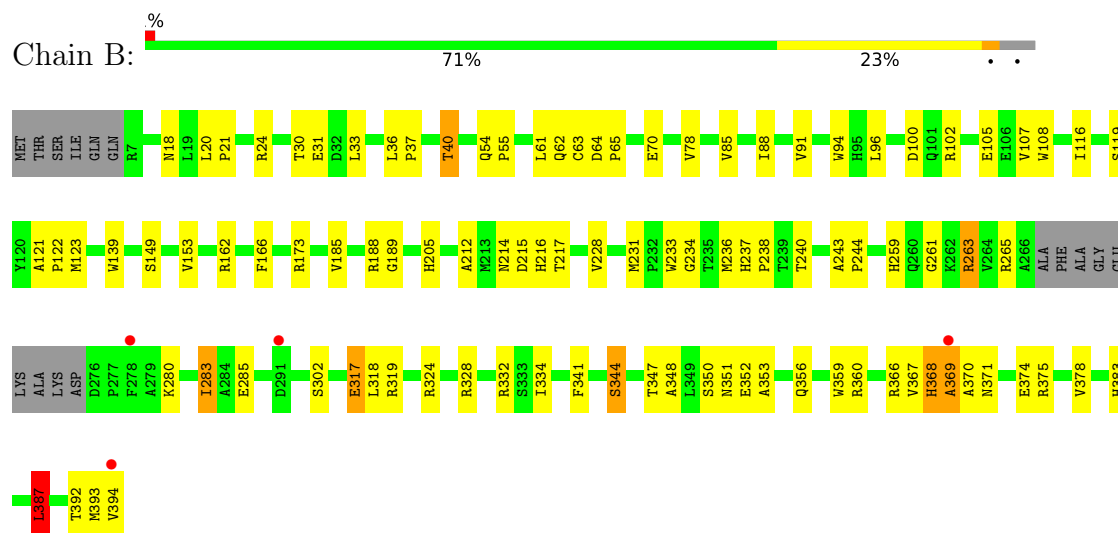
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

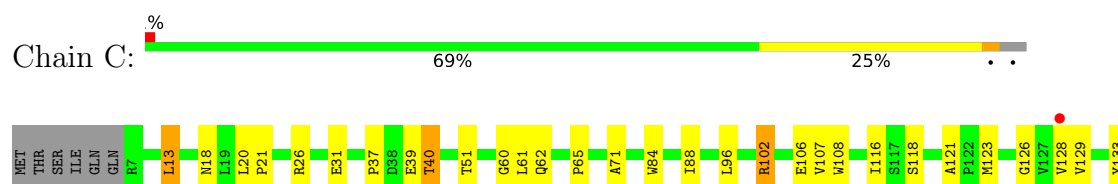
• Molecule 1: Hydroxylase, putative

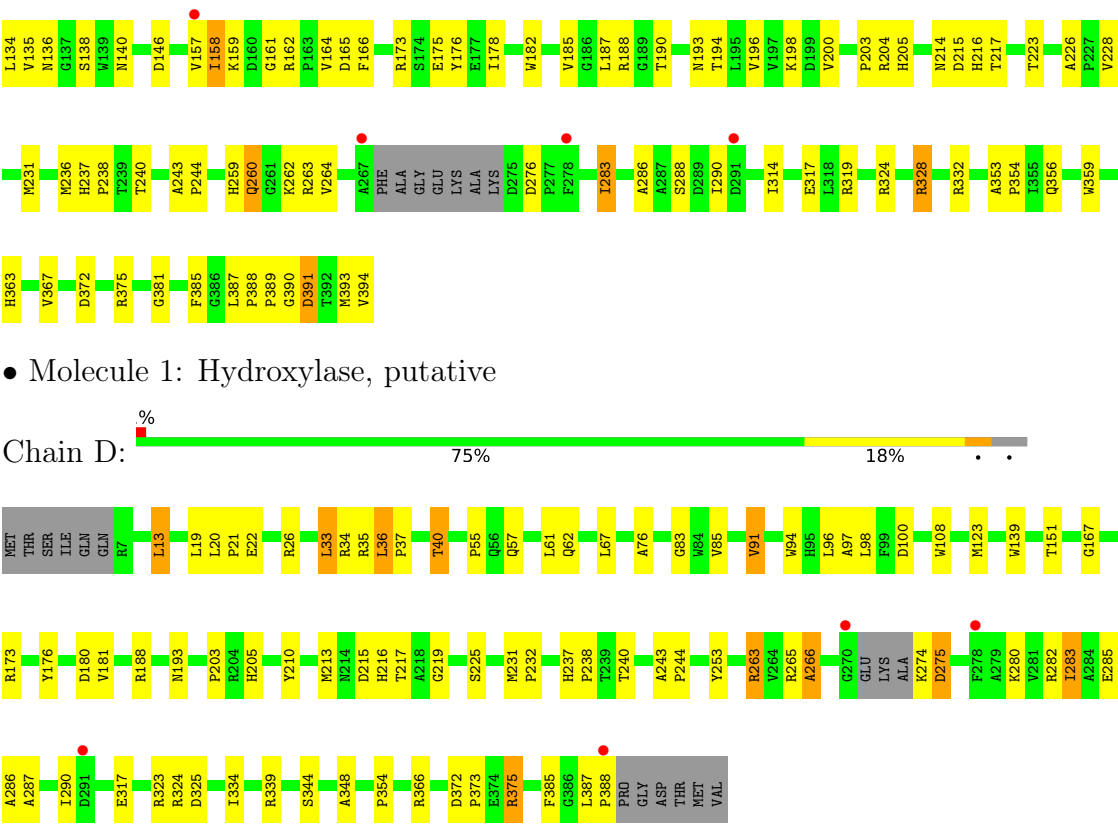


• Molecule 1: Hydroxylase, putative

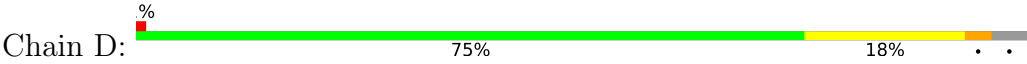


• Molecule 1: Hydroxylase, putative





● Molecule 1: Hydroxylase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.97Å 94.01Å 98.09Å 90.00° 93.94° 90.00°	Depositor
Resolution (Å)	28.80 – 2.50 28.80 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.80-2.50) 99.9 (28.80-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.191 , 0.258 0.186 , 0.251	Depositor DCC
R_{free} test set	2870 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 24.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12261	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/3047	0.82	1/4144 (0.0%)
1	B	0.48	0/3012	0.86	6/4099 (0.1%)
1	C	0.43	0/3025	0.80	2/4117 (0.0%)
1	D	0.45	0/3013	0.80	0/4098
All	All	0.45	0/12097	0.82	9/16458 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	LEU	CA-C-N	8.05	125.46	119.66
1	B	387	LEU	C-N-CA	8.05	125.46	119.66
1	C	314	ILE	N-CA-C	5.65	112.70	107.56
1	B	368	HIS	N-CA-C	-5.50	101.77	109.96
1	C	118	SER	N-CA-C	5.45	116.43	108.14
1	A	63	CYS	N-CA-C	5.21	116.81	110.41
1	B	63	CYS	N-CA-C	5.12	117.14	110.53
1	B	368	HIS	CA-C-N	5.03	130.75	121.70
1	B	368	HIS	C-N-CA	5.03	130.75	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2970	0	2869	68	0
1	B	2935	0	2833	85	0
1	C	2948	0	2842	85	0
1	D	2936	0	2833	56	0
2	A	158	0	0	8	1
2	B	114	0	0	6	0
2	C	90	0	0	12	0
2	D	110	0	0	5	0
All	All	12261	0	11377	285	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ARG:HH11	1:C:40:THR:HG22	1.12	1.12
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.18	1.05
1:B:231:MET:CB	1:B:236:MET:HE1	1.92	0.99
1:C:237:HIS:O	1:C:240:THR:HG22	1.63	0.97
1:B:231:MET:HB3	1:B:236:MET:HE1	1.47	0.96
1:B:368:HIS:HA	1:B:369:ALA:HB2	1.54	0.89
1:A:231:MET:HB3	1:A:236:MET:HE1	1.53	0.89
1:C:65:PRO:HG3	1:C:228:VAL:HG23	1.55	0.87
1:D:237:HIS:O	1:D:240:THR:HG22	1.74	0.87
1:A:236:MET:O	1:A:240:THR:HG22	1.75	0.86
1:C:214:ASN:HB3	2:C:410:HOH:O	1.75	0.85
1:C:328:ARG:HH11	1:C:328:ARG:CG	1.91	0.84
1:B:319:ARG:HH21	1:B:393:MET:CE	1.91	0.84
1:A:231:MET:HB3	1:A:236:MET:CE	2.07	0.83
1:A:98:LEU:HD12	1:A:213:MET:HE3	1.61	0.83
1:A:319:ARG:HH21	1:A:393:MET:CE	1.92	0.83
1:C:260:GLN:HE21	1:C:260:GLN:HA	1.45	0.81
1:C:121:ALA:HB3	1:C:123:MET:HE2	1.62	0.81
1:C:328:ARG:HH11	1:C:328:ARG:HG3	1.43	0.81
1:B:88:ILE:HG23	2:B:469:HOH:O	1.79	0.81
1:A:237:HIS:O	1:A:240:THR:HG23	1.81	0.81
1:B:368:HIS:HA	1:B:369:ALA:CB	2.09	0.80
1:B:65:PRO:HG3	1:B:228:VAL:HG23	1.64	0.80
1:D:263:ARG:HH11	1:D:263:ARG:HB3	1.48	0.78
1:B:263:ARG:HG2	1:B:263:ARG:HH11	1.46	0.77
1:B:368:HIS:ND1	1:B:369:ALA:HB3	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HG2	1:A:328:ARG:NH1	1.96	0.75
1:D:375:ARG:HG3	2:D:399:HOH:O	1.86	0.74
1:A:393:MET:HE3	2:A:546:HOH:O	1.87	0.74
1:B:185:VAL:HB	2:C:433:HOH:O	1.88	0.74
1:B:96:LEU:HD22	1:B:116:ILE:HD11	1.70	0.73
1:C:128:VAL:HG21	1:C:159:LYS:HB2	1.71	0.71
1:D:387:LEU:HB3	1:D:388:PRO:HD2	1.72	0.71
1:B:231:MET:CB	1:B:236:MET:CE	2.67	0.70
1:B:319:ARG:HH21	1:B:393:MET:HE1	1.56	0.69
1:C:237:HIS:O	1:C:240:THR:CG2	2.40	0.69
1:C:26:ARG:NH1	1:C:40:THR:HG22	1.97	0.69
1:C:231:MET:CB	1:C:236:MET:HE3	2.23	0.69
1:B:231:MET:HB3	1:B:236:MET:CE	2.22	0.68
1:B:214:ASN:HB3	2:B:447:HOH:O	1.93	0.68
1:B:121:ALA:HB3	1:B:123:MET:HE2	1.76	0.67
1:B:319:ARG:HH21	1:B:393:MET:HE2	1.59	0.67
1:C:182:TRP:HB2	1:C:193:ASN:ND2	2.09	0.67
1:A:98:LEU:HD12	1:A:213:MET:CE	2.24	0.67
1:C:353:ALA:O	1:C:356:GLN:HG3	1.94	0.67
1:B:215:ASP:HB3	1:B:217:THR:HG23	1.76	0.66
1:A:231:MET:HE3	1:A:236:MET:HE1	1.78	0.66
1:A:22:GLU:HG3	2:A:397:HOH:O	1.96	0.66
1:B:263:ARG:HH11	1:B:263:ARG:CG	2.08	0.66
1:C:96:LEU:HD23	1:C:108:TRP:CH2	2.31	0.65
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.00	0.65
1:B:392:THR:O	1:B:393:MET:HG2	1.96	0.65
1:B:231:MET:HB2	1:B:236:MET:HE1	1.77	0.64
1:B:319:ARG:HE	1:B:393:MET:HE1	1.63	0.64
1:D:203:PRO:HB2	1:D:205:HIS:CE1	2.33	0.64
1:A:328:ARG:HH12	1:B:285:GLU:HG2	1.62	0.64
1:B:231:MET:HB2	1:B:236:MET:CE	2.28	0.64
1:D:96:LEU:HD23	1:D:108:TRP:CH2	2.33	0.64
1:D:265:ARG:O	1:D:266:ALA:HB3	1.99	0.63
1:B:237:HIS:HB3	1:B:238:PRO:HD3	1.80	0.63
1:B:100:ASP:HB2	2:B:435:HOH:O	1.97	0.63
1:A:319:ARG:HE	1:A:393:MET:HE1	1.63	0.63
1:C:328:ARG:CG	1:C:328:ARG:NH1	2.58	0.63
1:D:334:ILE:HD11	1:D:366:ARG:HB2	1.81	0.62
1:C:319:ARG:HH21	1:C:394:VAL:C	2.07	0.62
1:C:237:HIS:HB3	1:C:238:PRO:HD3	1.81	0.62
1:C:260:GLN:O	1:C:264:VAL:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLY:O	1:C:162:ARG:HB2	1.99	0.62
1:A:321:ARG:HD3	2:A:414:HOH:O	2.00	0.61
1:C:354:PRO:HD2	2:C:407:HOH:O	2.00	0.61
1:B:280:LYS:O	1:B:283:ILE:HG22	1.99	0.61
1:D:243:ALA:HB3	1:D:244:PRO:HD3	1.82	0.61
1:B:102:ARG:HD2	1:B:205:HIS:NE2	2.16	0.61
1:B:215:ASP:O	1:B:216:HIS:HB2	1.99	0.61
1:D:57:GLN:HG2	2:D:469:HOH:O	2.01	0.60
1:D:181:VAL:H	1:D:193:ASN:ND2	1.99	0.60
1:A:319:ARG:HH21	1:A:393:MET:HE2	1.64	0.60
1:A:123:MET:HE1	1:A:140:ASN:OD1	2.00	0.60
1:A:319:ARG:HH21	1:A:393:MET:HE1	1.65	0.60
1:A:296:GLN:OE1	1:A:332:ARG:NH1	2.32	0.60
1:A:282:ARG:HD3	1:A:343:ALA:HB2	1.83	0.60
1:D:98:LEU:HD13	1:D:213:MET:HE3	1.83	0.59
1:B:91:VAL:HG11	1:B:240:THR:HG21	1.83	0.59
1:B:139:TRP:CE2	1:B:153:VAL:HB	2.37	0.59
1:B:234:GLY:HA3	1:B:393:MET:HG3	1.84	0.59
1:A:324:ARG:O	1:A:328:ARG:HB2	2.03	0.59
1:B:102:ARG:HD2	1:B:205:HIS:CD2	2.38	0.58
1:A:243:ALA:HB3	1:A:244:PRO:HD3	1.85	0.58
1:C:215:ASP:O	1:C:216:HIS:HB2	2.02	0.57
1:C:231:MET:HB2	1:C:236:MET:HE3	1.84	0.57
1:A:20:LEU:HB2	1:A:21:PRO:HD3	1.85	0.57
1:D:237:HIS:HB3	1:D:238:PRO:HD3	1.85	0.57
1:D:282:ARG:HD2	2:D:502:HOH:O	2.04	0.57
1:B:233:TRP:CD1	1:B:394:VAL:HG21	2.39	0.57
1:A:278:PHE:HD2	1:A:282:ARG:NH2	2.04	0.56
1:C:231:MET:HB3	1:C:236:MET:HE3	1.86	0.56
1:C:84:TRP:O	1:C:88:ILE:HG13	2.05	0.56
1:B:36:LEU:HD22	1:B:85:VAL:HG11	1.88	0.56
1:C:146:ASP:HA	2:C:430:HOH:O	2.05	0.56
1:A:98:LEU:HD21	1:A:229:TYR:HB3	1.86	0.56
1:A:181:VAL:H	1:A:193:ASN:ND2	2.03	0.56
1:C:259:HIS:HB2	2:C:472:HOH:O	2.05	0.56
1:D:354:PRO:HD2	2:D:397:HOH:O	2.06	0.56
1:B:356:GLN:HE22	1:B:360:ARG:HH21	1.53	0.55
1:C:106:GLU:OE1	1:C:205:HIS:NE2	2.35	0.55
1:C:26:ARG:HD2	1:C:40:THR:HG22	1.88	0.55
1:C:215:ASP:HB3	1:C:217:THR:HG23	1.86	0.55
1:A:231:MET:HB3	1:A:236:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LEU:HD22	1:B:116:ILE:CD1	2.36	0.55
1:A:328:ARG:NH1	1:A:328:ARG:CG	2.64	0.54
1:B:261:GLY:O	1:B:265:ARG:HD3	2.07	0.54
1:C:372:ASP:OD2	1:C:375:ARG:HB2	2.08	0.54
1:A:339:ARG:HD2	2:A:421:HOH:O	2.07	0.54
1:D:263:ARG:HH11	1:D:263:ARG:CB	2.19	0.54
1:A:233:TRP:CD1	1:A:394:VAL:HG21	2.42	0.54
1:B:107:VAL:HG12	1:B:108:TRP:CD1	2.42	0.54
1:B:344:SER:HB3	1:B:348:ALA:HB2	1.90	0.54
1:C:62:GLN:NE2	1:C:226:ALA:HB2	2.23	0.54
1:B:368:HIS:CA	1:B:369:ALA:CB	2.80	0.54
1:D:26:ARG:HH11	1:D:40:THR:HG22	1.72	0.53
1:D:215:ASP:HB3	1:D:217:THR:HG23	1.91	0.53
1:D:265:ARG:O	1:D:266:ALA:CB	2.56	0.53
1:D:96:LEU:HD23	1:D:108:TRP:CZ2	2.43	0.53
1:A:253:TYR:HA	1:A:340:LEU:HD13	1.90	0.53
1:B:263:ARG:CG	1:B:263:ARG:NH1	2.71	0.53
1:B:259:HIS:HD2	2:B:421:HOH:O	1.91	0.53
1:D:13:LEU:HD21	1:D:67:LEU:HB3	1.91	0.52
1:A:260:GLN:HE22	1:A:263:ARG:CZ	2.21	0.52
1:B:236:MET:O	1:B:240:THR:HG23	2.10	0.52
1:A:334:ILE:CD1	1:A:366:ARG:HB2	2.40	0.52
1:D:286:ALA:O	1:D:290:ILE:HG13	2.10	0.52
1:D:253:TYR:CE1	1:D:287:ALA:HB2	2.44	0.52
1:D:334:ILE:CD1	1:D:366:ARG:HB2	2.39	0.52
1:B:96:LEU:HD23	1:B:108:TRP:CZ2	2.45	0.51
1:C:203:PRO:HB2	1:C:205:HIS:CE1	2.46	0.51
1:D:181:VAL:H	1:D:193:ASN:HD22	1.57	0.51
1:B:319:ARG:NH2	1:B:393:MET:HE1	2.24	0.51
1:C:96:LEU:HD23	1:C:108:TRP:CZ2	2.46	0.51
1:B:368:HIS:CG	1:B:369:ALA:HB3	2.45	0.51
1:B:96:LEU:HD23	1:B:108:TRP:CH2	2.46	0.51
1:C:204:ARG:HG3	2:C:402:HOH:O	2.11	0.51
1:C:215:ASP:CB	1:C:217:THR:HG23	2.42	0.50
1:C:288:SER:HB2	1:D:324:ARG:HD2	1.94	0.50
1:C:328:ARG:O	1:C:332:ARG:HG2	2.11	0.50
1:C:166:PHE:HB3	2:C:418:HOH:O	2.12	0.50
1:B:359:TRP:CZ2	1:C:359:TRP:CZ2	2.99	0.49
1:C:173:ARG:HA	1:C:176:TYR:CZ	2.47	0.49
1:B:243:ALA:HB3	1:B:244:PRO:HD3	1.94	0.49
1:A:173:ARG:HA	1:A:176:TYR:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ARG:HD2	1:C:40:THR:CG2	2.42	0.48
1:D:36:LEU:HD22	1:D:85:VAL:HG11	1.95	0.48
1:D:34:ARG:HA	1:D:188:ARG:O	2.12	0.48
1:A:364:ALA:O	1:A:367:VAL:HG22	2.13	0.48
1:B:185:VAL:O	1:B:360:ARG:HD2	2.13	0.48
1:C:31:GLU:HG3	1:C:188:ARG:HB2	1.94	0.48
1:A:51:THR:HB	1:A:60:GLY:HA2	1.96	0.48
1:C:231:MET:HE3	1:C:236:MET:HE1	1.96	0.48
1:C:39:GLU:HB2	2:C:455:HOH:O	2.14	0.48
1:C:166:PHE:CB	2:C:418:HOH:O	2.61	0.48
1:D:167:GLY:HA2	1:D:210:TYR:CD1	2.49	0.48
1:A:173:ARG:NH2	2:A:442:HOH:O	2.47	0.47
1:C:381:GLY:HA3	1:D:280:LYS:HB3	1.95	0.47
1:C:126:GLY:CA	1:C:135:VAL:HG22	2.44	0.47
1:B:280:LYS:O	1:B:283:ILE:CG2	2.62	0.47
1:C:136:ASN:OD1	1:C:198:LYS:HA	2.14	0.47
1:D:100:ASP:HB3	1:D:219:GLY:HA3	1.97	0.47
1:B:280:LYS:C	1:B:283:ILE:HG22	2.39	0.47
1:C:231:MET:CE	1:C:236:MET:HE1	2.44	0.47
1:C:283:ILE:HD12	1:D:385:PHE:CZ	2.49	0.47
1:A:334:ILE:HD11	1:A:366:ARG:HB2	1.97	0.47
1:A:182:TRP:HB2	1:A:193:ASN:ND2	2.30	0.47
1:C:178:ILE:HD13	2:C:430:HOH:O	2.15	0.47
1:B:317:GLU:HB2	1:B:383:HIS:CE1	2.50	0.46
1:B:334:ILE:CD1	1:B:366:ARG:HB2	2.46	0.46
1:A:277:PRO:O	1:A:281:VAL:HG23	2.15	0.46
1:B:91:VAL:O	1:B:94:TRP:HB3	2.15	0.46
1:B:341:PHE:HE1	1:B:356:GLN:HB3	1.80	0.46
1:C:175:GLU:O	1:C:200:VAL:HG21	2.15	0.46
1:C:328:ARG:HH12	1:D:285:GLU:HA	1.80	0.46
1:C:102:ARG:O	1:C:106:GLU:HG3	2.14	0.46
1:C:107:VAL:HG12	1:C:108:TRP:CD1	2.51	0.46
1:C:385:PHE:CZ	1:D:283:ILE:HD13	2.51	0.46
1:B:31:GLU:HG3	1:B:188:ARG:HB2	1.98	0.46
1:B:319:ARG:NE	1:B:393:MET:HE1	2.29	0.46
1:C:61:LEU:O	1:C:62:GLN:C	2.58	0.46
1:B:356:GLN:NE2	1:B:360:ARG:HH21	2.14	0.46
1:B:20:LEU:HB2	1:B:21:PRO:HD3	1.97	0.46
1:A:236:MET:CA	1:A:236:MET:HE2	2.45	0.45
1:A:312:LYS:HE2	1:A:312:LYS:HB3	1.73	0.45
1:A:253:TYR:CE1	1:A:287:ALA:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HD12	1:C:13:LEU:HA	1.64	0.45
1:B:37:PRO:HD2	1:B:40:THR:CG2	2.47	0.45
1:C:138:SER:OG	1:C:196:VAL:HG22	2.17	0.45
1:D:344:SER:HB3	1:D:348:ALA:HB2	1.98	0.45
1:D:167:GLY:HA2	1:D:210:TYR:CE1	2.52	0.45
1:B:374:GLU:O	1:B:378:VAL:HG23	2.17	0.45
1:C:123:MET:HE1	1:C:140:ASN:OD1	2.17	0.45
1:B:18:ASN:O	1:B:21:PRO:HD2	2.17	0.44
1:C:20:LEU:HB2	1:C:21:PRO:HD3	1.99	0.44
1:C:243:ALA:HB3	1:C:244:PRO:HD3	1.98	0.44
1:C:286:ALA:O	1:C:290:ILE:HG13	2.16	0.44
1:A:233:TRP:NE1	1:A:394:VAL:HG21	2.32	0.44
1:C:276:ASP:HB3	2:C:434:HOH:O	2.16	0.44
1:A:173:ARG:NH1	2:A:518:HOH:O	2.44	0.44
1:A:328:ARG:HG2	1:A:377:TYR:OH	2.16	0.44
1:C:37:PRO:HB2	1:C:40:THR:HG23	1.99	0.44
1:A:14:ALA:O	1:A:17:ASP:HB2	2.18	0.44
1:A:179:LYS:O	1:A:193:ASN:HB3	2.17	0.44
1:D:324:ARG:HG3	1:D:325:ASP:N	2.32	0.44
1:B:328:ARG:HD3	2:B:451:HOH:O	2.18	0.44
1:D:215:ASP:O	1:D:216:HIS:HB2	2.18	0.44
1:B:122:PRO:HB3	1:B:166:PHE:CZ	2.53	0.43
1:D:180:ASP:HA	1:D:193:ASN:ND2	2.33	0.43
1:B:317:GLU:HG3	1:B:318:LEU:N	2.33	0.43
1:D:387:LEU:CB	1:D:388:PRO:HD2	2.46	0.43
1:C:185:VAL:HG22	1:C:185:VAL:O	2.19	0.43
1:C:332:ARG:NH1	2:C:408:HOH:O	2.04	0.43
1:C:133:TYR:HE1	1:C:157:VAL:CG1	2.31	0.43
1:B:65:PRO:HG3	1:B:228:VAL:CG2	2.41	0.43
1:D:20:LEU:HB2	1:D:21:PRO:HD3	1.99	0.43
1:B:236:MET:HB2	1:B:236:MET:HE2	1.55	0.43
1:C:385:PHE:CZ	1:D:283:ILE:CD1	3.02	0.43
1:A:386:GLY:HA2	2:A:476:HOH:O	2.19	0.43
1:C:128:VAL:CG2	1:C:159:LYS:HB2	2.45	0.43
1:C:260:GLN:HA	1:C:260:GLN:NE2	2.23	0.43
1:D:36:LEU:HA	1:D:37:PRO:HD3	1.93	0.43
1:D:274:LYS:O	1:D:275:ASP:HB3	2.19	0.43
1:A:182:TRP:CZ2	1:A:184:VAL:HG21	2.53	0.42
1:A:177:GLU:OE2	1:A:179:LYS:HE3	2.19	0.42
1:D:19:LEU:O	1:D:22:GLU:HG2	2.19	0.42
1:D:123:MET:HE3	1:D:139:TRP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:MET:HB3	1:C:236:MET:CE	2.47	0.42
1:C:388:PRO:HA	1:C:389:PRO:HD3	1.87	0.42
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.93	0.42
1:C:187:LEU:HB3	1:C:190:THR:CG2	2.49	0.42
1:A:26:ARG:O	1:A:27:ALA:C	2.62	0.42
1:B:36:LEU:HA	1:B:37:PRO:HD3	1.95	0.42
1:C:262:LYS:HG3	1:C:263:ARG:H	1.84	0.42
1:B:212:ALA:HA	1:B:215:ASP:HB2	2.00	0.42
1:D:91:VAL:O	1:D:94:TRP:HB3	2.20	0.42
1:D:151:THR:HG22	1:D:176:TYR:CE2	2.54	0.42
1:C:126:GLY:HA2	1:C:135:VAL:HG22	2.01	0.42
1:A:124:GLY:HA3	1:A:139:TRP:CZ2	2.54	0.42
1:A:319:ARG:NH2	1:A:393:MET:HE1	2.33	0.42
1:D:55:PRO:HG3	1:D:97:ALA:HB2	2.01	0.42
1:D:372:ASP:HA	1:D:373:PRO:HD3	1.88	0.42
1:C:231:MET:CB	1:C:236:MET:CE	2.96	0.42
1:D:61:LEU:O	1:D:62:GLN:C	2.62	0.42
1:B:328:ARG:O	1:B:332:ARG:HG3	2.20	0.41
1:C:390:GLY:O	1:C:391:ASP:C	2.63	0.41
1:D:339:ARG:NE	2:D:418:HOH:O	2.53	0.41
1:A:54:GLN:HB3	1:A:60:GLY:HA3	2.00	0.41
1:B:70:GLU:HB2	2:B:418:HOH:O	2.21	0.41
1:B:350:SER:C	1:B:352:GLU:H	2.28	0.41
1:A:88:ILE:O	1:A:91:VAL:HG12	2.20	0.41
1:A:285:GLU:HB3	1:B:328:ARG:HH21	1.85	0.41
1:B:392:THR:C	1:B:393:MET:HG2	2.45	0.41
1:B:353:ALA:O	1:B:356:GLN:HG3	2.20	0.41
1:C:18:ASN:HD22	1:C:18:ASN:HA	1.66	0.41
1:A:234:GLY:HA3	1:A:393:MET:SD	2.61	0.41
1:A:282:ARG:CD	1:A:343:ALA:HB2	2.48	0.41
1:B:387:LEU:HA	1:B:387:LEU:HD12	1.72	0.41
1:D:76:ALA:HB2	1:D:83:GLY:HA3	2.03	0.41
1:B:24:ARG:HB2	1:B:78:VAL:HB	2.03	0.41
1:A:181:VAL:H	1:A:193:ASN:HD22	1.67	0.41
1:A:353:ALA:O	1:A:356:GLN:HG3	2.20	0.41
1:B:30:THR:HG22	1:B:189:GLY:HA3	2.03	0.41
1:B:61:LEU:O	1:B:62:GLN:C	2.64	0.41
1:C:158:ILE:HG13	1:C:162:ARG:O	2.21	0.41
1:D:33:LEU:O	1:D:34:ARG:HB2	2.21	0.41
1:A:277:PRO:HD2	2:A:475:HOH:O	2.20	0.41
1:A:350:SER:OG	1:A:352:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLN:HA	1:B:55:PRO:HD3	1.95	0.41
1:C:51:THR:HB	1:C:60:GLY:HA2	2.03	0.41
1:D:231:MET:HA	1:D:232:PRO:HD3	1.92	0.41
1:A:236:MET:HE2	1:A:236:MET:N	2.36	0.40
1:A:118:SER:HA	1:A:152:PHE:O	2.22	0.40
1:B:64:ASP:OD1	1:B:64:ASP:C	2.63	0.40
1:C:236:MET:CA	1:C:236:MET:HE2	2.50	0.40
1:A:237:HIS:HA	1:A:240:THR:CG2	2.50	0.40
1:B:119:SER:OG	1:B:139:TRP:HB3	2.20	0.40
1:C:359:TRP:O	1:C:363:HIS:HD2	2.05	0.40
1:D:26:ARG:HH11	1:D:40:THR:CG2	2.34	0.40
1:B:368:HIS:O	1:B:371:ASN:HB2	2.20	0.40
1:C:13:LEU:HD11	1:C:71:ALA:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:485:HOH:O	2:A:551:HOH:O[2_645]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/394 (96%)	371 (98%)	5 (1%)	2 (0%)	24	43
1	B	375/394 (95%)	357 (95%)	15 (4%)	3 (1%)	16	31
1	C	377/394 (96%)	356 (94%)	20 (5%)	1 (0%)	36	55
1	D	375/394 (95%)	360 (96%)	13 (4%)	2 (0%)	24	43
All	All	1505/1576 (96%)	1444 (96%)	53 (4%)	8 (0%)	24	43

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	351	ASN
1	B	369	ALA
1	D	266	ALA
1	A	269	ALA
1	C	391	ASP
1	A	393	MET
1	B	370	ALA
1	D	275	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/310 (97%)	288 (96%)	13 (4%)	26	51
1	B	299/310 (96%)	283 (95%)	16 (5%)	20	41
1	C	300/310 (97%)	281 (94%)	19 (6%)	16	34
1	D	297/310 (96%)	284 (96%)	13 (4%)	25	50
All	All	1197/1240 (96%)	1136 (95%)	61 (5%)	21	43

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	179	LYS
1	A	198	LYS
1	A	204	ARG
1	A	214	ASN
1	A	236	MET
1	A	240	THR
1	A	283	ILE
1	A	324	ARG
1	A	328	ARG
1	A	352	GLU
1	A	375	ARG
1	A	392	THR
1	B	33	LEU

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Mol	Chain	Res	Type
1	B	40	THR
1	B	105	GLU
1	B	149	SER
1	B	162	ARG
1	B	173	ARG
1	B	263	ARG
1	B	283	ILE
1	B	302	SER
1	B	317	GLU
1	B	324	ARG
1	B	344	SER
1	B	347	THR
1	B	367	VAL
1	B	375	ARG
1	B	387	LEU
1	C	13	LEU
1	C	40	THR
1	C	102	ARG
1	C	116	ILE
1	C	129	VAL
1	C	134	LEU
1	C	158	ILE
1	C	164	VAL
1	C	165	ASP
1	C	194	THR
1	C	223	THR
1	C	260	GLN
1	C	283	ILE
1	C	317	GLU
1	C	324	ARG
1	C	328	ARG
1	C	367	VAL
1	C	387	LEU
1	C	393	MET
1	D	13	LEU
1	D	33	LEU
1	D	35	ARG
1	D	36	LEU
1	D	40	THR
1	D	91	VAL
1	D	173	ARG
1	D	225	SER

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Mol	Chain	Res	Type
1	D	263	ARG
1	D	283	ILE
1	D	317	GLU
1	D	323	ARG
1	D	375	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	57	GLN
1	A	101	GLN
1	A	193	ASN
1	A	224	ASN
1	A	259	HIS
1	A	260	GLN
1	A	300	ASN
1	A	371	ASN
1	B	193	ASN
1	B	260	GLN
1	B	300	ASN
1	B	356	GLN
1	B	383	HIS
1	C	18	ASN
1	C	57	GLN
1	C	101	GLN
1	C	193	ASN
1	C	224	ASN
1	C	237	HIS
1	C	260	GLN
1	C	300	ASN
1	C	371	ASN
1	D	18	ASN
1	D	193	ASN
1	D	214	ASN
1	D	300	ASN
1	D	371	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	384/394 (97%)	-0.48	2 (0%) 87 85	16, 32, 51, 76	1 (0%)
1	B	379/394 (96%)	-0.43	4 (1%) 78 75	18, 35, 57, 77	1 (0%)
1	C	381/394 (96%)	-0.04	5 (1%) 75 71	19, 45, 69, 89	1 (0%)
1	D	379/394 (96%)	-0.39	4 (1%) 78 75	19, 36, 60, 93	1 (0%)
All	All	1523/1576 (96%)	-0.34	15 (0%) 79 76	16, 37, 63, 93	4 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	GLY	3.7
1	B	394	VAL	3.6
1	C	267	ALA	3.1
1	A	278	PHE	2.8
1	C	278	PHE	2.7
1	B	291	ASP	2.6
1	C	291	ASP	2.6
1	B	278	PHE	2.5
1	B	369	ALA	2.4
1	A	392	THR	2.3
1	D	278	PHE	2.3
1	C	157	VAL	2.3
1	D	388	PRO	2.2
1	C	128	VAL	2.1
1	D	291	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.